Scientific software engineering for a simple ODE model

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List of Exercises and Problems

Goal.

This document illustrates *best practice* for developing scientific software in an efficient and reliable way. Not only will the outlined techniques save a lost of human time, but they will also help assure reproducible science and higher quality of computational investigations. Key questions to be answered are

- How should I organize a program?
- How can I efficiently and safely provide input data and run my code?
- How can I verify that the implementation is correct?
- How should I reliably work with files and documents?
- How should I conduct large numerical experiments?

hpl 1: Need to cover functions, classes, modules, cml, GUI, hand calc, trivial problems, exact num sol, MMS, qualitative results, Git, bitbucket/github, scripting, report generation

1 Sample problem and code

This first introduction to good programming habits in scientific computing will make use of a very simple mathematical problem to keep the mathematical details at the lowest possible level while introducing a series of computer science concepts. The simplicity of the mathematical problem obviously prevents us from treating several techniques that are only meaningful for complex scientific software.

1.1 Mathematical problem

We consider the simplest possible ordinary differential equation with constant coefficient a:

$$u'(t) = -au(t), \quad u(0) = I, \quad t \in (0, T]\,. \tag{1}$$

This problem is numerically solved by the so-called θ-rule, which is a convenient way to merge different formulas for the well-known Forward Euler, Backward Euler, and Crank-Nicolson (midpoint/central) schemes. We introduce a uniform time mesh $t_n = n\Delta t$, $n = 0, 1, \ldots, N_t$, and seek $u(t)$ at the mesh points. The numerical approximation to $u(t_n)$ is denoted u^n. Since we will use the symbol u both for the exact analytical solution of (1) and for the numerical

approximation, we sometimes introduce $u_{\mathrm{e}}(t)$ to help distinguish the two types of solutions (i.e., subscript e for "exact")[1].

The θ-rule leads to an explicit updating formula for u^{n+1}, given u^n:

$$u^{n+1} = \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}u^n,$$

1.2 Implementation

The numerical method is implemented as a function `solver`. Another function `explore` computes the error in the solution, by comparing with the exact solution $u_{\mathrm{e}}(t) = Ie^{-at}$, and creates a plot for comparing the numerical and exact solution.

The program file `decay_plot.py` contains the two functions and a main program.

```
from numpy import *
from matplotlib.pyplot import *

def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    dt = float(dt)            # avoid integer division
    Nt = int(round(T/dt))     # no of time intervals
    T = Nt*dt                 # adjust T to fit time step dt
    u = zeros(Nt+1)           # array of u[n] values
    t = linspace(0, T, Nt+1)  # time mesh

    u[0] = I                  # assign initial condition
    for n in range(0, Nt):    # n=0,1,...,Nt-1
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t

def exact_solution(t, I, a):
    return I*exp(-a*t)

def explore(I, a, T, dt, theta=0.5, makeplot=True):
    """
    Run a case with the solver, compute error measure,
    and plot the numerical and exact solutions (if makeplot=True).
    """
    u, t = solver(I, a, T, dt, theta)    # Numerical solution
    u_e = exact_solution(t, I, a)
    e = u_e - u
    E = sqrt(dt*sum(e**2))
    if makeplot:
        figure()                         # create new plot
        t_e = linspace(0, T, 1001)       # fine mesh for u_e
        u_e = exact_solution(t_e, I, a)
        plot(t,   u,   'r--o')           # red dashes w/circles
        plot(t_e, u_e, 'b-')             # blue line for exact sol.
        legend(['numerical', 'exact'])
```

[1] In the literature, it is more common to put a subscript (like u_Δ or u_h) on the numerical solution to distinguish it from the exact solution. However, we will use the variable `u` in the code for the numerical approximation to be computed, and therefore adjust the mathematical notation to convenient conventions in the code such that we can have as close correspondence as possible between the implementation and the mathematics.

```
        xlabel('t')
        ylabel('u')
        title('theta=%g, dt=%g' % (theta, dt))
        theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
        savefig('%s_%g.png' % (theta2name[theta], dt))
        savefig('%s_%g.pdf' % (theta2name[theta], dt))
        show()
    return E

def main(I, a, T, dt_values, theta_values=(0, 0.5, 1)):
    for theta in theta_values:
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot=True)
            print '%3.1f %6.2f: %12.3E' % (theta, dt, E)

main(I=1, a=2, T=5, dt_values=[0.4, 0.04])
```

2 User interfaces

It is good programming practice to let programs read input from the user rather than require the user to edit the source code when trying out new values of input parameters. One reason is that any edit of the code has a danger of introducing bugs. Another reason is that it is easier and less manual work to supply data to a program instead of editing the program code. A third reason is that a program that reads input can easily be run by another program, and in this way we can automate a large number of runs in scientific investigations.

Tip.

We shall make it a habit to equip any implementation of a numerical solver with an appropriate user interface before testing out the code.

Reading input data can be done in many ways. We have to decide on desired *user interface*, i.e., how we want to operate the program when providing input, and then use appropriate tools to implement the user interface. There are four basic types of user interface of relevance to our programs, listed here with increasing complexity of the implementation:

1. Questions and answers in the terminal window
2. Command-line arguments
3. Reading data from file
4. Graphical user interfaces

Although conceptually simple, alternative 1 involves more typing than the other alternatives and is therefore abandoned. Below, we shall address alternative 2 and 4, which are most appropriate for the present problem.

[[[

2.1 Creating command-line interfaces

Reading input from the command line is a simple and flexible way of interacting with the user. Python stores all the command-line arguments in the list `sys.argv`, and there are, in principle, two ways of programming with command-line arguments in Python:

- Decide upon a sequence of parameters on the command line and read their values directly from the `sys.argv[1:]` list (`sys.argv[0]` is the just program name).
- Use option-value pairs (`-option value`) on the command line to override default values of input parameters, and utilize the `argparse.ArgumentParser` tool to interact with the command line.

Both strategies will be illustrated next.

Reading a sequence of command-line arguments. The `decay_plot.py` program needs the following input data: I, a, T, an option to turn the plot on or off (`makeplot`), and a list of Δt values.

The simplest way of reading this input from the command line is to say that the first four command-line arguments correspond to the first four points in the list above, in that order, and that the rest of the command-line arguments are the Δt values. The input given for `makeplot` can be a string among `'on'`, `'off'`, `'True'`, and `'False'`. The code for reading this input is most conveniently put in a function:

```
import sys

def read_command_line():
    if len(sys.argv) < 6:
        print 'Usage: %s I a T on/off dt1 dt2 dt3 ...' % \
              sys.argv[0]; sys.exit(1)  # abort

    I = float(sys.argv[1])
    a = float(sys.argv[2])
    T = float(sys.argv[3])
    makeplot = sys.argv[4] in ('on', 'True')
    dt_values = [float(arg) for arg in sys.argv[5:]]

    return I, a, T, makeplot, dt_values
```

One should note the following about the constructions in the program above:

- Everything on the command line ends up in a *string* in the list `sys.argv`. Explicit conversion to, e.g., a `float` object is required if the string as a number we want to compute with.
- The value of `makeplot` is determined from a boolean expression, which becomes `True` if the command-line argument is either `'on'` or `'True'`, and `False` otherwise.

- It is easy to build the list of Δt values: we simply run through the rest of the list, `sys.argv[5:]`, convert each command-line argument to `float`, and collect these `float` objects in a list, using the compact and convenient *list comprehension* syntax in Python.

The loops over θ and Δt values can be coded in a `main` function:

```
def main():
    I, a, T, makeplot, dt_values = read_command_line()
    for theta in 0, 0.5, 1:
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot)
            print '%3.1f %6.2f: %12.3E' % (theta, dt, E)
```

The complete program can be found in `decay_cml.py`.

Working with an argument parser. Python's `ArgumentParser` tool in the `argparse` module makes it easy to create a professional command-line interface to any program. The documentation of `ArgumentParser` demonstrates its versatile applications, so we shall here just list an example containing basic features. On the command line we want to specify option-value pairs for I, a, and T, e.g., `-a 3.5 -I 2 -T 2`. Including `-makeplot` turns the plot on and excluding this option turns the plot off. The Δt values can be given as `-dt 1 0.5 0.25 0.1 0.01`. Each parameter must have a sensible default value so that we specify the option on the command line only when the default value is not suitable.

We introduce a function for defining the mentioned command-line options:

```
def define_command_line_options():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument('--I', '--initial_condition', type=float,
                        default=1.0, help='initial condition, u(0)',
                        metavar='I')
    parser.add_argument('--a', type=float,
                        default=1.0, help='coefficient in ODE',
                        metavar='a')
    parser.add_argument('--T', '--stop_time', type=float,
                        default=1.0, help='end time of simulation',
                        metavar='T')
    parser.add_argument('--makeplot', action='store_true',
                        help='display plot or not')
    parser.add_argument('--dt', '--time_step_values', type=float,
                        default=[1.0], help='time step values',
                        metavar='dt', nargs='+', dest='dt_values')
    return parser
```

Each command-line option is defined through the `parser.add_argument` method. Alternative options, like the short `-I` and the more explaining version `--initial_condition` can be defined. Other arguments are `type` for the Python object type, a default value, and a help string, which gets printed if the command-line argument `-h` or `-help` is included. The `metavar` argument specifies the

value associated with the option when the help string is printed. For example, the option for I has this help output:

```
Terminal> python decay_argparse.py -h
  ...
  --I I, --initial_condition I
                        initial condition, u(0)
  ...
```

The structure of this output is

```
      --I metavar, --initial_condition metavar
                           help-string
```

The `-makeplot` option is a pure flag without any value, implying a true value if the flag is present and otherwise a false value. The `action='store_true'` makes an option for such a flag.

Finally, the `-dt` option demonstrates how to allow for more than one value (separated by blanks) through the `nargs='+'` keyword argument. After the command line is parsed, we get an object where the values of the options are stored as attributes. The attribute name is specified by the `dist` keyword argument, which for the `-dt` option is `dt_values`. Without the `dest` argument, the value of an option `-opt` is stored as the attribute `opt`.

The code below demonstrates how to read the command line and extract the values for each option:

```
def read_command_line():
    parser = define_command_line_options()
    args = parser.parse_args()
    print 'I={}, a={}, T={}, makeplot={}, dt_values={}'.format(
        args.I, args.a, args.T, args.makeplot, args.dt_values)
    return args.I, args.a, args.T, args.makeplot, args.dt_values
```

The `main` function remains the same as in the `decay_cml.py` code based on reading from `sys.argv` directly. A complete program featuring the demo above of `ArgumentParser` appears in the file `decay_argparse.py`.

2.2 Creating a graphical web user interface

The Python package Parampool can be used to automatically generate a web-based *graphical user interface* (GUI) for our simulation program. Although the programming technique dramatically simplifies the efforts to create a GUI, the forthcoming material on equipping our `decay_mod` module with a GUI is quite technical and of significantly less importance than knowing how to make a command-line interface (Section 2.1). There is no danger in jumping right to Section 3.4.

Making a compute function. The first step is to identify a function that performs the computations and that takes the necessary input variables as arguments. This is called the *compute function* in Parampool terminology. We may start with a copy of the basic file `decay_plot.py`, which has a `main` function displayed in Section **??** for carrying out simulations and plotting for a series of Δt values. Now we want to control and view the same experiments from a web GUI.

To tell Parampool what type of input data we have, we assign default values of the right type to all arguments in the main function and call it `main_GUI`:

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
```

The compute function must return the HTML code we want for displaying the result in a web page. Here we want to show plots of the numerical and exact solution for different methods and Δt values. The plots can be organized in a table with θ (methods) varying through the columns and Δt varying through the rows. Assume now that a new version of the `explore` function not only returns the error `E` but also HTML code containing the plot. Then we can write the `main_GUI` function as

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
    # Build HTML code for web page. Arrange plots in columns
    # corresponding to the theta values, with dt down the rows
    theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
    html_text = '<table>\n'
    for dt in dt_values:
        html_text += '<tr>\n'
        for theta in theta_values:
            E, html = explore(I, a, T, dt, theta, makeplot=True)
            html_text += """
<td>
<center><b>%s, dt=%g, error: %s</b></center><br>
%s
</td>
""" % (theta2name[theta], dt, E, html)
        html_text += '</tr>\n'
    html_text += '</table>\n'
    return html_text
```

Rather than creating plot files and showing the plot on the screen, the new version of the `explore` function makes a string with the PNG code of the plot and embeds that string in HTML code. This action is conveniently performed by Parampool's `save_png_to_str` function:

```
import matplotlib.pyplot as plt
...
# plot
plt.plot(t, u, r-')
plt.xlabel('t')
```

```
plt.ylabel('u')
...
from parampool.utils import save_png_to_str
html_text = save_png_to_str(plt, plotwidth=400)
```

Note that we now write `plt.plot`, `plt.xlabel`, etc. The `html_text` string is long and contains all the characters that build up the PNG file of the current plot. The new `explore` function can make use of the above code snippet and return `html_text` along with `E`.

Generating the user interface. The web GUI is automatically generated by the following code, placed in a file `decay_GUI_generate.py`

```
from parampool.generator.flask import generate
from decay_GUI import main
generate(main,
         output_controller='decay_GUI_controller.py',
         output_template='decay_GUI_view.py',
         output_model='decay_GUI_model.py')
```

Running the `decay_GUI_generate.py` program results in three new files whose names are specified in the call to `generate`:

1. `decay_GUI_model.py` defines HTML widgets to be used to set input data in the web interface,
2. `templates/decay_GUI_views.py` defines the layout of the web page,
3. `decay_GUI_controller.py` runs the web application.

We only need to run the last program, and there is no need to look into these files.

Running the web application. The web GUI is started by

```
Terminal> python decay_GUI_controller.py
```

Open a web browser at the location `127.0.0.1:5000`. Input fields for `I`, `a`, `T`, `dt_values`, and `theta_values` are presented. Setting the latter two to `[1.25, 0.5]` and `[1, 0.5]`, respectively, and pressing *Compute* results in four plots, see Figure 1. With the techniques demonstrated here, one can easily create a tailored web GUI for a particular type of application and use it to interactively explore physical and numerical effects.

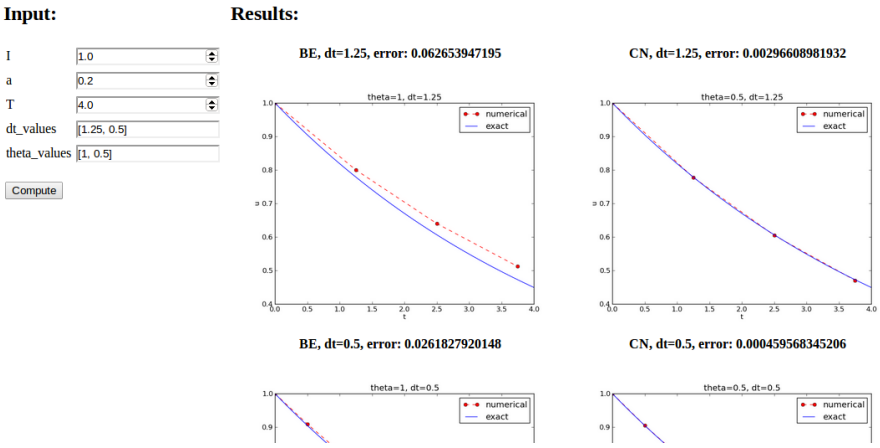


Figure 1: Automatically generated graphical web interface.

3 Verification

3.1 Comparison with hand calculations

One of the simplest and most powerful methods for verifying numerical codes is to perform some steps of the algorithm by hand and compare the results with those produced by the code. In the present case, we may choose some test problem and run three steps by hand. Picking $a(t) = t^2$... **hpl 2**: Not ready. Time-dep a?

3.2 Test function

Caution: choice of parameter values.

For the choice of values of parameters in verification tests one should stay away from integers, especially 0 and 1, as these can simplify formulas too much for test purposes. For example, with $\theta = 1$ the nominator in the formula for u^n will be the same for all a and Δt values. One should therefore choose more "arbitrary" values, say $\theta = 0.8$ and $I = 0.1$.

3.3 Comparison with an exact discrete solution

Sometimes it is possible to find a closed-form *exact discrete solution* that fulfills the discrete finite difference equations. The implementation can then be verified against the exact discrete solution. This is usually the best technique for verification.

Define

$$A = \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}\,.$$

Manual computations with the θ-rule results in

$$\begin{aligned} u^0 &= I,\\ u^1 &= Au^0 = AI,\\ u^2 &= Au^1 = A^2 I,\\ &\vdots\\ u^n &= A^n u^{n-1} = A^n I\,. \end{aligned}$$

We have then established the exact discrete solution as

$$u^n = IA^n\,. \tag{2}$$

Caution.

One should be conscious about the different meanings of the notation on the left- and right-hand side of (2): on the left, n in u^n is a superscript reflecting a counter of mesh points (t_n), while on the right, n is the power in the exponentiation A^n.

Comparison of the exact discrete solution and the computed solution is done in the following function:

```
def verify_exact_discrete_solution():

    def exact_discrete_solution(n, I, a, theta, dt):
        A = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
        return I*A**n

    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    Nt = int(8/dt)  # no of steps
    u, t = solver(I=I, a=a, T=Nt*dt, dt=dt, theta=theta)
    u_de = array([exact_discrete_solution(n, I, a, theta, dt)
                  for n in range(Nt+1)])
    difference = abs(u_de - u).max()  # max deviation
    tol = 1E-15  # tolerance for comparing floats
    success = difference <= tol
    return success
```

The complete program is found in the file `decay_verf2.py` (`verf2` is a short name for "verification, version 2").

Local functions.

One can define a function inside another function, here called a *local function* (also known as *closure*) inside a *parent function*. A local function is invisible outside the parent function. A convenient property is that any local function has access to all variables defined in the parent function, also if we send the local function to some other function as argument (!). In the present example, it means that the local function `exact_discrete_solution` does not need its five arguments as the values can alternatively be accessed through the local variables defined in the parent function `verify_exact_discrete_solution`. We can send such an `exact_discrete_solution` without arguments to any other function and `exact_discrete_solution` will still have access to `n`, `I`, `a`, and so forth defined in its parent function.

3.4 Computing convergence rates

We expect that the error E in the numerical solution is reduced if the mesh size Δt is decreased. More specifically, many numerical methods obey a power-law relation between E and Δt:

$$E = C\Delta t^r, \tag{3}$$

where C and r are (usually unknown) constants independent of Δt. The formula (3) is viewed as an asymptotic model valid for sufficiently small Δt. How small is normally hard to estimate without doing numerical estimations of r.

The parameter r is known as the *convergence rate*. For example, if the convergence rate is 2, halving Δt reduces the error by a factor of 4. Diminishing Δt then has a greater impact on the error compared with methods that have $r = 1$. For a given value of r, we refer to the method as of r-th order. First- and second-order methods are most common in scientific computing.

Estimating r. There are two alternative ways of estimating C and r based on a set of m simulations with corresponding pairs $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$, and $\Delta t_i < \Delta t_{i-1}$ (i.e., decreasing cell size).

1. Take the logarithm of (3), $\ln E = r \ln \Delta t + \ln C$, and fit a straight line to the data points $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$.
2. Consider two consecutive experiments, $(\Delta t_i, E_i)$ and $(\Delta t_{i-1}, E_{i-1})$. Dividing the equation $E_{i-1} = C\Delta t_{i-1}^r$ by $E_i = C\Delta t_i^r$ and solving for r yields

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \tag{4}$$

for $i = 1, \ldots, m-1$.

The disadvantage of method 1 is that (3) might not be valid for the coarsest meshes (largest Δt values). Fitting a line to all the data points is then misleading. Method 2 computes convergence rates for pairs of experiments and allows us to see if the sequence r_i converges to some value as $i \to m-2$. The final r_{m-2} can then be taken as the convergence rate. If the coarsest meshes have a differing rate, the corresponding time steps are probably too large for (3) to be valid. That is, those time steps lie outside the asymptotic range of Δt values where the error behaves like (3).

Implementation. It is straightforward to extend the `main` function in the program `decay_argparse.py` with statements for computing $r_0, r_1, \ldots, r_{m-2}$ from (3):

```
from math import log

def main():
    I, a, T, makeplot, dt_values = read_command_line()
    r = {}  # estimated convergence rates
    for theta in 0, 0.5, 1:
        E_values = []
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot=False)
            E_values.append(E)

        # Compute convergence rates
        m = len(dt_values)
        r[theta] = [log(E_values[i-1]/E_values[i])/
                    log(dt_values[i-1]/dt_values[i])
                    for i in range(1, m, 1)]

    for theta in r:
        print '\nPairwise convergence rates for theta=%g:' % theta
        print ' '.join(['%.2f' % r_ for r_ in r[theta]])
    return r
```

The program containing this `main` function is called `decay_convrate.py`.

The `r` object is a *dictionary of lists*. The keys in this dictionary are the θ values. For example, `r[1]` holds the list of the r_i values corresponding to $\theta = 1$. In the loop `for theta in r`, the loop variable `theta` takes on the values of the keys in the dictionary `r` (in an undetermined ordering). We could simply do a `print r[theta]` inside the loop, but this would typically yield output of the convergence rates with 16 decimals:

```
[1.331919482274763, 1.1488178494691532, ...]
```

Instead, we format each number with 2 decimals, using a list comprehension to turn the list of numbers, `r[theta]`, into a list of formatted strings. Then we join these strings with a space in between to get a sequence of rates on one line in the terminal window. More generally, `d.join(list)` joins the strings in the list `list` to one string, with `d` as delimiter between `list[0]`, `list[1]`, etc.

Here is an example on the outcome of the convergence rate computations:

```
Terminal> python decay_convrate.py --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.33 1.15 1.07 1.03 1.02

Pairwise convergence rates for theta=0.5:
2.14 2.07 2.03 2.01 2.01

Pairwise convergence rates for theta=1:
0.98 0.99 0.99 1.00 1.00
```

The Forward and Backward Euler methods seem to have an r value which stabilizes at 1, while the Crank-Nicolson seems to be a second-order method with $r = 2$.

Very often, we have some theory that predicts what r is for a numerical method. Various theoretical error measures for the θ-rule point to $r = 2$ for $\theta = 0.5$ and $r = 1$ otherwise. The computed estimates of r are in very good agreement with these theoretical values.

Why convergence rates are important.

The strong practical application of computing convergence rates is for verification: wrong convergence rates point to errors in the code, and correct convergence rates brings evidence that the implementation is correct. Experience shows that bugs in the code easily destroy the expected convergence rate.

Debugging via convergence rates. Let us experiment with bugs and see the implication on the convergence rate. We may, for instance, forget to multiply by `a` in the denominator in the updating formula for `u[n+1]`:

```
u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt)*u[n]
```

Running the same `decay_convrate.py` command as above gives the expected convergence rates (!). Why? The reason is that we just specified the Δt values are relied on default values for other parameters. The default value of a is 1. Forgetting the factor `a` has then no effect. This example shows how important it is to avoid parameters that are 1 or 0 when verifying implementations. Running the code `decay_v0.py` with $a = 2.1$ and $I = 0.1$ yields

```
Terminal> python decay_convrate.py --a 2.1 --I 0.1  \
          --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.49 1.18 1.07 1.04 1.02
```

```
Pairwise convergence rates for theta=0.5:
-1.42 -0.22 -0.07 -0.03 -0.01

Pairwise convergence rates for theta=1:
0.21 0.12 0.06 0.03 0.01
```

This time we see that the expected convergence rates for the Crank-Nicolson and Backward Euler methods are not obtained, while $r = 1$ for the Forward Euler method. The reason for correct rate in the latter case is that $\theta = 0$ and the wrong `theta*dt` term in the denominator vanishes anyway.

The error

```
u[n+1] = ((1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
```

manifests itself through wrong rates $r \approx 0$ for all three methods. About the same results arise from an erroneous initial condition, `u[0] = 1`, or wrong loop limits, `range(1,Nt)`. It seems that in this simple problem, most bugs we can think of are detected by the convergence rate test, provided the values of the input data do not hide the bug.

A `verify_convergence_rate` function could compute the dictionary of list via `main` and check if the final rate estimates (r_{m-2}) are sufficiently close to the expected ones. A tolerance of 0.1 seems appropriate, given the uncertainty in estimating r:

```
def verify_convergence_rate():
    r = main()
    tol = 0.1
    expected_rates = {0: 1, 1: 1, 0.5: 2}
    for theta in r:
        r_final = r[theta][-1]
        diff = abs(expected_rates[theta] - r_final)
        if diff > tol:
            return False
    return True  # all tests passed
```

We remark that `r[theta]` is a list and the last element in any list can be extracted by the index `-1`.

4 Software engineering

Goal.

Efficient use of differential equation models requires software that is easy to test and flexible for setting up extensive numerical experiments. This section introduces three important concepts:

- Modules

- Testing frameworks
- Implementation with classes

The concepts are introduced using the differential equation problem $u' = -au$, $u(0) = I$, as example.

4.1 Making a module

The DRY principle.

The previous sections have outlined numerous different programs, all of them having their own copy of the `solver` function. Such copies of the same piece of code is against the important *Don't Repeat Yourself* (DRY) principle in programming. If we want to change the `solver` function there should be *one and only one* place where the change needs to be performed.

To clean up the repetitive code snippets scattered among the `decay_*.py` files, we start by collecting the various functions we want to keep for the future in one file, now called `decay_mod.py` (`mod` stands for "module"). The following functions are copied to this file:

- `solver` for computing the numerical solution
- `verify_three_steps` for verifying the first three solution points against hand calculations
- `verify_discrete_solution` for verifying the entire computed solution against an exact formula for the numerical solution
- `explore` for computing and plotting the solution
- `define_command_line_options` for defining option-value pairs on the command line
- `read_command_line` for reading input from the command line, now extended to work both with `sys.argv` directly and with an `ArgumentParser` object
- `main` for running experiments with $\theta = 0, 0.5, 1$ and a series of Δt values, and computing convergence rates
- `main_GUI` for doing the same as the `main` function, but modified for automatic GUI generation
- `verify_convergence_rate` for verifying the computed convergence rates against the theoretically expected values

We use Matplotlib for plotting. A sketch of the `decay_mod.py` file, with complete versions of the modified functions, looks as follows:

```
from numpy import *
from matplotlib.pyplot import *
import sys

def solver(I, a, T, dt, theta):
    ...

def verify_three_steps():
    ...

def verify_exact_discrete_solution():
    ...

def u_exact(t, I, a):
    ...

def explore(I, a, T, dt, theta=0.5, makeplot=True):
    ...

def define_command_line_options():
    ...

def read_command_line(use_argparse=True):
    if use_argparse:
        parser = define_command_line_options()
        args = parser.parse_args()
        print 'I={}, a={}, makeplot={}, dt_values={}'.format(
            args.I, args.a, args.makeplot, args.dt_values)
        return args.I, args.a, args.makeplot, args.dt_values
    else:
        if len(sys.argv) < 6:
            print 'Usage: %s I a on/off dt1 dt2 dt3 ...' % \
                  sys.argv[0]; sys.exit(1)

        I = float(sys.argv[1])
        a = float(sys.argv[2])
        T = float(sys.argv[3])
        makeplot = sys.argv[4] in ('on', 'True')
        dt_values = [float(arg) for arg in sys.argv[5:]]

        return I, a, makeplot, dt_values

def main():
    ...
```

This `decay_mod.py` file is already a module such that we can import desired functions in other programs. For example, we can in a file do

```
from decay_mod import solver
u, t = solver(I=1.0, a=3.0, T=3, dt=0.01, theta=0.5)
```

However, it should also be possible to both use `decay_mod.py` as a module *and* execute the file as a program that runs `main()`. This is accomplished by ending the file with a *test block*:

```
if __name__ == '__main__':
    main()
```

When `decay_mod.py` is used as a module, `__name__` equals the module name `decay_mod`, while `__name__` equals `'__main__'` when the file is run as a program. Optionally, we could run the verification tests if the word `verify` is present on the command line and `verify_convergence_rate` could be tested if `verify_rates` is found on the command line. The `verify_rates` argument must be removed before we read parameter values from the command line, otherwise the `read_command_line` function (called by `main`) will not work properly.

```
if __name__ == '__main__':
    if 'verify' in sys.argv:
        if verify_three_steps() and verify_discrete_solution():
            pass # ok
        else:
            print 'Bug in the implementation!'
    elif 'verify_rates' in sys.argv:
        sys.argv.remove('verify_rates')
        if not '--dt' in sys.argv:
            print 'Must assign several dt values'
            sys.exit(1)  # abort
        if verify_convergence_rate():
            pass
        else:
            print 'Bug in the implementation!'
    else:
        # Perform simulations
        main()
```

4.2 Prefixing imported functions by the module name

Import statements of the form `from module import *` import functions and variables in `module.py` into the current file. For example, when doing

```
from numpy import *
from matplotlib.pyplot import *
```

we get mathematical functions like `sin` and `exp` as well as MATLAB-style functions like `linspace` and `plot`, which can be called by these well-known names. Unfortunately, it sometimes becomes confusing to know where a particular function comes from. Is it from `numpy`? Or `matplotlib.pyplot`? Or is it our own function?

An alternative import is

```
import numpy
import matplotlib.pyplot
```

and such imports require functions to be prefixed by the module name, e.g.,

```
t = numpy.linspace(0, T, Nt+1)
u_e = I*numpy.exp(-a*t)
matplotlib.pyplot.plot(t, u_e)
```

This is normally regarded as a better habit because it is explicitly stated from which module a function comes from.

The modules `numpy` and `matplotlib.pyplot` are so frequently used, and their full names quite tedious to write, so two standard abbreviations have evolved in the Python scientific computing community:

```
import numpy as np
import matplotlib.pyplot as plt

t = np.linspace(0, T, Nt+1)
u_e = I*np.exp(-a*t)
plt.plot(t, u_e)
```

A version of the `decay_mod` module where we use the `np` and `plt` prefixes is found in the file `decay_mod_prefix.py`.

The downside of prefixing functions by the module name is that mathematical expressions like $e^{-at}\sin(2\pi t)$ get cluttered with module names,

```
numpy.exp(-a*t)*numpy.sin(2(numpy.pi*t)
# or
np.exp(-a*t)*np.sin(2*np.pi*t)
```

Such an expression looks like `exp(-a*t)*sin(2*pi*t)` in most other programming languages. Similarly, `np.linspace` and `plt.plot` look less familiar to people who are used to MATLAB and who have not adopted Python's prefix style. Whether to do `from module import *` or `import module` depends on personal taste and the problem at hand. In these writings we use `from module import` in shorter programs where similarity with MATLAB could be an advantage, and where a one-to-one correspondence between mathematical formulas and Python expressions is important. The style `import module` is preferred inside Python modules (see Exercise 5 for a demonstration).

4.3 Doctests

We have emphasized how important it is to be able to run tests in the program at any time. This was solved by calling various `verify*` functions in the previous examples. However, there exists well-established procedures and corresponding tools for automating the execution of tests. We shall briefly demonstrate two important techniques: *doctest* and *unit testing*. The corresponding files are the modules `decay_mod_doctest.py` and `decay_mod_nosetest.py`.

A doc string (the first string after the function header) is used to document the purpose of functions and their arguments. Very often it is instructive to include an example on how to use the function. Interactive examples in the Python shell are most illustrative as we can see the output resulting from function

calls. For example, we can in the `solver` function include an example on calling this function and printing the computed `u` and `t` arrays:

```
def solver(I, a, T, dt, theta):
    """
    Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt.


    >>> u, t = solver(I=0.8, a=1.2, T=4, dt=0.5, theta=0.5)
    >>> for t_n, u_n in zip(t, u):
    ...     print 't=%.1f, u=%.14f' % (t_n, u_n)
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
    t=2.5, u=0.03621291001985
    t=3.0, u=0.01949925924146
    t=3.5, u=0.01049960113002
    t=4.0, u=0.00565363137770
    """
    ...
```

When such interactive demonstrations are inserted in doc strings, Python's `doctest` module can be used to automate running all commands in interactive sessions and compare new output with the output appearing in the doc string. All we have to do in the current example is to write

```
Terminal> python -m doctest decay_mod_doctest.py
```

This command imports the `doctest` module, which runs all tests. No additional command-line argument is allowed when running doctests. If any test fails, the problem is reported, e.g.,

```
Terminal> python -m doctest decay_mod_doctest.py
**********************************************************
File "decay_mod_doctest.py", line 12, in decay_mod_doctest....
Failed example:
    for t_n, u_n in zip(t, u):
        print 't=%.1f, u=%.14f' % (t_n, u_n)
Expected:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
Got:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254718756
**********************************************************
1 items had failures:
   1 of   2 in decay_mod_doctest.solver
***Test Failed*** 1 failures.
```

Note that in the output of `t` and `u` we write `u` with 14 digits. Writing all 16 digits is not a good idea: if the tests are run on different hardware, round-off errors might be different, and the `doctest` module detects that the numbers are not precisely the same and reports failures. In the present application, where $0 < u(t) \leq 0.8$, we expect round-off errors to be of size 10^{-16}, so comparing 15 digits would probably be reliable, but we compare 14 to be on the safe side.

Doctests are highly encouraged as they do two things: 1) demonstrate how a function is used and 2) test that the function works.

Here is an example on a doctest in the `explore` function:

```
def explore(I, a, T, dt, theta=0.5, makeplot=True):
    """
    Run a case with the solver, compute error measure,
    and plot the numerical and exact solutions (if makeplot=True).

    >>> for theta in 0, 0.5, 1:
    ...     E = explore(I=1.9, a=2.1, T=5, dt=0.1, theta=theta,
    ...                 makeplot=False)
    ...     print '%.10E' % E
    ...
    7.3565079236E-02
    2.4183893110E-03
    6.5013039886E-02
    """
    ...
```

This time we limit the output to 10 digits.

Caution.

Doctests requires careful coding if they use command-line input or print results to the terminal window. Command-line input must be simulated by filling `sys.argv` correctly, e.g., `sys.argv = '-I 1.0 -a 5'.split`. The output lines of print statements must be copied exactly as they appear when running the statements in an interactive Python shell.

4.4 Unit testing with nose

The unit testing technique consists of identifying small units of code, usually functions (or classes), and write one or more tests for each unit. One test should, ideally, not depend on the outcome of other tests. For example, the doctest in function `solver` is a unit test, and the doctest in function `explore` as well, but the latter depends on a working `solver`. Putting the error computation and plotting in `explore` in two separate functions would allow independent unit tests. In this way, the design of unit tests impacts the design of functions. The recommended practice is actually to design and write the unit tests first and *then* implement the functions!

In scientific computing it is not always obvious how to best perform unit testing. The units is naturally larger than in non-scientific software. Very often the solution procedure of a mathematical problem identifies a unit.

Basic use of nose. The `nose` package is a versatile tool for implementing unit tests in Python. Here is a short explanation of the usage of nose:

1. Implement tests in functions with names starting with `test_`. Such functions cannot have any arguments.
2. The test functions perform assertions on computed results using `assert` functions from the `nose.tools` module.
3. The test functions can be in the source code files or be collected in separate files with names `test*.py`.

Here comes a very simple illustration of the three points. Assume that we have this function in a module `mymod`:

```
def double(n):
    return 2*n
```

Either in this file, or in a separate file `test_mymod.py`, we implement a test function whose purpose is to test that the function `double` works as intended:

```
import nose.tools as nt

def test_double():
    result = double(4)
    nt.assert_equal(result, 8)
```

Notice that `test_double` has no arguments. We need to do an `import mymod` or `from mymod import double` if this test resides in a separate file. Running

```
Terminal> nosetests -s mymod
```

makes the `nose` tool run all functions with names matching `test_*()` in `mymod.py`. Alternatively, if the test functions are in some `test_mymod.py` file, we can just write `nosetests -s`. The nose tool will then look for all files with names mathching `test*.py` and run all functions `test_*()` in these files.

When you have nose tests in separate test files with names `test*.py` it is common to collect these files in a subdirectory `tests`, or `*_tests` if you have several test subdirectories. Running `nosetests -s` will then recursively look for all `tests` and `*_tests` subdirectories and run all functions `test_*()` in all files `test_*.py` in these directories. Just one command can then launch a series of tests in a directory tree!

An example of a `tests` directory with different types of `test*.py` files are found in src/decay/tests. Note that these perform imports of modules in the parent directory. These imports works well because the tests are supposed to be run by `nosetests -s` executed in the parent directory (`decay`).

Tip.

The `-s` option to `nosetests` assures that any print statement in the `test_*` functions appears in the output. Without this option, `nosetests` suppressed whatever the tests writes to the terminal window (standard output). Such behavior is annoying, especially when developing and testing tests.

The number of failed tests and their details are reported, or an `OK` is printed if all tests passed.

The advantage with the `nose` package is two-fold:

1. tests are written and collected in a structured way, and
2. large collections of tests, scattered throughout a tree of directories, can be executed with one command `nosetests -s`.

Alternative assert statements. In case the `nt.assert_equal` function finds that the two arguments are equal, the test is a success, otherwise it is a failure and an exception of type `AssertionError` is raised. The particular exception is the indicator that a test has failed.

Instead of calling the convenience function `nt.assert_equal`, we can use Python's plain `assert` statement, which tests if a boolean expression is true and raises an `AssertionError` otherwise. Here, the statement is `assert result == 8`.

A completely manual alternative is to explicitly raise an `AssertionError` exception if the computed result is wrong:

```
if result != 8:
    raise AssertionError()
```

Applying nose. Let us illustrate how to use the `nose` tool for testing key functions in the `decay_mod` module. Or more precisely, the module is called `decay_mod_unittest` with all the `verify*` functions removed as these now are outdated by the unit tests.

We design three unit tests:

1. A comparison between the computed u^n values and the exact discrete solution.
2. A comparison between the computed u^n values and precomputed, verified reference values.
3. A comparison between observed and expected convergence rates.

These tests follow very closely the code in the previously shown `verify*` functions. We start with comparing u^n, as computed by the function `solver`, to the formula for the exact discrete solution:

```
import nose.tools as nt
import decay_mod_unittest as decay_mod
import numpy as np

def exact_discrete_solution(n, I, a, theta, dt):
    """Return exact discrete solution of the theta scheme."""
    dt = float(dt)  # avoid integer division
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

def test_exact_discrete_solution():
    """
    Compare result from solver against
    formula for the discrete solution.
    """
    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    N = int(8/dt)  # no of steps
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

The `nt.assert_almost_equal` is the relevant function for comparing two real numbers. The `delta` argument specifies a tolerance for the comparison. Alternatively, one can specify a `places` argument for the number of decimal places to be used in the comparison.

After having carefully verified the implementation, we may store correctly computed numbers in the test program or in files for use in future tests. Here is an example on how the outcome from the `solver` function can be compared to what is considered to be correct results:

```
def test_solver():
    """
    Compare result from solver against
    precomputed arrays for theta=0, 0.5, 1.
    """
    I=0.8; a=1.2; T=4; dt=0.5  # fixed parameters
    precomputed = {
        't': np.array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5,
                        3. ,  3.5,  4. ]),
        0.5: np.array(
            [ 0.8       ,  0.43076923,  0.23195266, 0.12489759,
              0.06725255,  0.03621291,  0.01949926, 0.0104996 ,
              0.00565363]),
        0: np.array(
            [  8.00000000e-01,   3.20000000e-01,
               1.28000000e-01,   5.12000000e-02,
               2.04800000e-02,   8.19200000e-03,
               3.27680000e-03,   1.31072000e-03,
               5.24288000e-04]),
        1: np.array(
```

```
            [ 0.8       ,  0.5       ,  0.3125    ,  0.1953125 ,
              0.12207031,  0.07629395,  0.04768372,  0.02980232,
              0.01862645]),
        }
    for theta in 0, 0.5, 1:
        u, t = decay_mod.solver(I, a, T, dt, theta=theta)
        diff = np.abs(u - precomputed[theta]).max()
        # Precomputed numbers are known to 8 decimal places
        nt.assert_almost_equal(diff, 0, places=8,
                               msg='theta=%s' % theta)
```

The `precomputed` object is a dictionary with four keys: `'t'` for the time mesh, and three θ values for u^n solutions corresponding to $\theta = 0, 0.5, 1$.

Testing for special type of input data that may cause trouble constitutes a common way of constructing unit tests. For example, the updating formula for u^{n+1} may be incorrectly evaluated because of unintended integer divisions. With

```
theta = 1; a = 1; I = 1; dt = 2
```

the nominator and denominator in the updating expression,

```
(1 - (1-theta)*a*dt)
(1 + theta*dt*a)
```

evaluate to 1 and 3, respectively, and the fraction `1/3` will call up integer division and consequently lead to `u[n+1]=0`. We construct a unit test to make sure `solver` is smart enough to avoid this problem:

```
def test_potential_integer_division():
    """Choose variables that can trigger integer division."""
    theta = 1; a = 1; I = 1; dt = 2
    N = 4
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

The final test is to see that the convergence rates corresponding to $\theta = 0, 0.5, 1$ are 1, 2, and 1, respectively:

```
def test_convergence_rates():
    """Compare empirical convergence rates to exact ones."""
    # Set command-line arguments directly in sys.argv
    import sys
    sys.argv[1:] = '--I 0.8 --a 2.1 --T 5 '\
                   '--dt 0.4 0.2 0.1 0.05 0.025'.split()
    r = decay_mod.main()
    for theta in r:
        nt.assert_true(r[theta])  # check for non-empty list

    expected_rates = {0: 1, 1: 1, 0.5: 2}
    for theta in r:
```

```
        r_final = r[theta][-1]
        # Compare to 1 decimal place
        nt.assert_almost_equal(expected_rates[theta], r_final,
                               places=1, msg='theta=%s' % theta)
```

Nothing more is needed in the `test_decay_nose.py` file where the tests reside. Running `nosetests -s` will report `Ran 3 tests` and an `OK` for success. Every time we modify the `decay_mod_unittest` module we can run `nosetests` to quickly see if the edits have any impact on the verification tests.

Installation of nose. The `nose` package does not come with a standard Python distribution and must therefore be installed separately. The procedure is standard and described on Nose's web pages. On Debian-based Linux systems the command is `sudo apt-get install python-nose`, and with MacPorts you run `sudo port install py27-nose`.

Using nose to test modules with doctests. Assume that `mod` is the name of some module that contains doctests. We may let `nose` run these doctests and report errors in the standard way using the code set-up

```
import doctest
import mod

def test_mod():
    failure_count, test_count = doctest.testmod(m=mod)
    nt.assert_equal(failure_count, 0,
                    msg='%d tests out of %d failed' %
                    (failure_count, test_count))
```

The call to `doctest.testmod` runs all doctests in the module file `mod.py` and returns the number of failures (`failure_count`) and the total number of tests (`test_count`). A real example is found in the file `test_decay_doctest.py`.

4.5 Classical class-based unit testing

The classical way of implementing unit tests derives from the JUnit tool in Java where all tests are methods in a class for testing. Python comes with a module `unittest` for doing this type of unit tests. While `nose` allows simple functions for unit tests, `unittest` requires deriving a class `Test*` from `unittest.TestCase` and implementing each test as methods with names `test_*` in that class. I strongly recommend to use `nose` over `unittest`, because it is much simpler and more convenient, but class-based unit testing is a very classical subject that computational scientists should have some knowledge about. That is why a short introduction to `unittest` is included below.

Basic use of unittest. We apply the `double` function in the `mymod` module introduced in the previous section as example. Unit testing with the aid of the `unittest` module consists of writing a file `test_mymod.py` with the content

```
import unittest
import mymod

class TestMyCode(unittest.TestCase):
    def test_double(self):
        result = mymod.double(4)
        self.assertEqual(result, 8)

if __name__ == '__main__':
    unittest.main()
```

The test is run by executing the test file `test_mymod.py` as a standard Python program. There is no support in `unittest` for automatically locating and running all tests in all test files in a directory tree.

Those who have experience with object-oriented programming will see that the difference between using `unittest` and `nose` is minor.

Demonstration of unittest. The same tests as shown for the nose framework are reimplemented with the `TestCase` classes in the file `test_decay_unittest.py`. The tests are identical, the only difference being that with `unittest` we must write the tests as methods in a class and the assert functions have slightly different names.

```
import unittest
import decay_mod_unittest as decay
import numpy as np

def exact_discrete_solution(n, I, a, theta, dt):
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

class TestDecay(unittest.TestCase):

    def test_exact_discrete_solution(self):
        ...
        diff = np.abs(u_de - u).max()
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_solver(self):
        ...
        for theta in 0, 0.5, 1:
            ...
            self.assertAlmostEqual(diff, 0, places=8,
                                   msg='theta=%s' % theta)

    def test_potential_integer_division():
        ...
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_convergence_rates(self):
        ...
        for theta in r:
            ...
            self.assertAlmostEqual(...)
```

```
if __name__ == '__main__':
    unittest.main()
```

4.6 Implementing simple problem and solver classes

The θ-rule was compactly and conveniently implemented in a function `solver` in Section **??**. In more complicated problems it might be beneficial to use classes and introduce a class `Problem` to hold the definition of the physical problem, a class `Solver` to hold the data and methods needed to numerically solve the problem, and a class `Visualizer` to make plots. This idea will now be illustrated, resulting in code that represents an alternative to the `solver` and `explore` functions found in the `decay_mod` module.

Explaining the details of class programming in Python is considered beyond the scope of this text. Readers who are unfamiliar with Python class programming should first consult one of the many electronic Python tutorials or textbooks to come up to speed with concepts and syntax of Python classes before reading on. The author has a gentle introduction to class programming for scientific applications in [1], see Chapter 7 and 9 and Appendix E. Other useful resources are

- The Python Tutorial: http://docs.python.org/2/tutorial/classes.html
- Wiki book on Python Programming: http://en.wikibooks.org/wiki/Python_Programming/Classes
- tutorialspoint.com: http://www.tutorialspoint.com/python/python_classes_objects.htm

The problem class. The purpose of the problem class is to store all information about the mathematical model. This usually means all the physical parameters in the problem. In the current example with exponential decay we may also add the exact solution of the ODE to the problem class. The simplest form of a problem class is therefore

```
from numpy import exp

class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def u_exact(self, t):
        I, a = self.I, self.a
        return I*exp(-a*t)
```

We could in the `u_exact` method have written `self.I*exp(-self.a*t)`, but using local variables `I` and `a` allows the formula `I*exp(-a*t)` which looks closer

to the mathematical expression Ie^{-at}. This is not an important issue with the current compact formula, but is beneficial in more complicated problems with longer formulas to obtain the closest possible relationship between code and mathematics. My coding style is to strip off the `self` prefix when the code expresses mathematical formulas.

The class data can be set either as arguments in the constructor or at any time later, e.g.,

```
problem = Problem(T=5)
problem.T = 8
problem.dt = 1.5
```

(Some programmers prefer `set` and `get` functions for setting and getting data in classes, often implemented via *properties* in Python, but I consider that overkill when we just have a few data items in a class.)

It would be convenient if class `Problem` could also initialize the data from the command line. To this end, we add a method for defining a set of command-line options and a method that sets the local attributes equal to what was found on the command line. The default values associated with the command-line options are taken as the values provided to the constructor. Class `Problem` now becomes

```
class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()

        parser.add_argument(
            '--I', '--initial_condition', type=float,
            default=self.I, help='initial condition, u(0)',
            metavar='I')
        parser.add_argument(
            '--a', type=float, default=self.a,
            help='coefficient in ODE', metavar='a')
        parser.add_argument(
            '--T', '--stop_time', type=float, default=self.T,
            help='end time of simulation', metavar='T')
        return parser

    def init_from_command_line(self, args):
        self.I, self.a, self.T = args.I, args.a, args.T

    def exact_solution(self, t):
        I, a = self.I, self.a
        return I*exp(-a*t)
```

Observe that if the user already has an `ArgumentParser` object it can be supplied, but if she does not have any, class `Problem` makes one. Python's `None` object is used to indicate that a variable is not initialized with a proper value.

The solver class. The solver class stores data related to the numerical solution method and provides a function `solve` for solving the problem. A problem object must be given to the constructor so that the solver can easily look up physical data. In the present example, the data related to the numerical solution method consists of Δt and θ. We add, as in the problem class, functionality for reading Δt and θ from the command line:

```
class Solver:
    def __init__(self, problem, dt=0.1, theta=0.5):
        self.problem = problem
        self.dt, self.theta = float(dt), theta

    def define_command_line_options(self, parser):
        parser.add_argument(
            '--dt', '--time_step_value', type=float,
            default=0.5, help='time step value', metavar='dt')
        parser.add_argument(
            '--theta', type=float, default=0.5,
            help='time discretization parameter', metavar='dt')
        return parser

    def init_from_command_line(self, args):
        self.dt, self.theta = args.dt, args.theta

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.I, self.problem.a, self.problem.T,
            self.dt, self.theta)

    def error(self):
        u_e = self.problem.exact_solution(self.t)
        e = u_e - self.u
        E = sqrt(self.dt*sum(e**2))
        return E
```

Note that we here simply reuse the implementation of the numerical method from the `decay_mod` module. The `solve` function is just a *wrapper* of the previously developed stand-alone `solver` function.

The visualizer class. The purpose of the visualizer class is to plot the numerical solution stored in class `Solver`. We also add the possibility to plot the exact solution. Access to the problem and solver objects is required when making plots so the constructor must hold references to these objects:

```
class Visualizer:
    def __init__(self, problem, solver):
        self.problem, self.solver = problem, solver

    def plot(self, include_exact=True, plt=None):
        """
        Add solver.u curve to the plotting object plt,
        and include the exact solution if include_exact is True.
        This plot function can be called several times (if
        the solver object has computed new solutions).
```

```
        """
        if plt is None:
            import scitools.std  as plt # can use matplotlib as well

        plt.plot(self.solver.t, self.solver.u, '--o')
        plt.hold('on')
        theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
        name = theta2name.get(self.solver.theta, '')
        legends = ['numerical %s' % name]
        if include_exact:
            t_e = linspace(0, self.problem.T, 1001)
            u_e = self.problem.exact_solution(t_e)
            plt.plot(t_e, u_e, 'b-')
            legends.append('exact')
        plt.legend(legends)
        plt.xlabel('t')
        plt.ylabel('u')
        plt.title('theta=%g, dt=%g' %
                  (self.solver.theta, self.solver.dt))
        plt.savefig('%s_%g.png' % (name, self.solver.dt))
        return plt
```

The `plt` object in the `plot` method is worth a comment. The idea is that `plot` can add a numerical solution curve to an existing plot. Calling `plot` with a `plt` object (which has to be a `matplotlib.pyplot` or `scitools.std` object in this implementation), will just add the curve `self.solver.u` as a dashed line with circles at the mesh points (leaving the color of the curve up to the plotting tool). This functionality allows plots with several solutions: just make a loop where new data is set in the problem and/or solver classes, the solver's `solve()` method is called, and the most recent numerical solution is plotted by the `plot(plt)` method in the visualizer object Exercise 6 describes a problem setting where this functionality is explored.

Combining the objects. Eventually we need to show how the classes `Problem`, `Solver`, and `Visualizer` play together:

```
def main():
    problem = Problem()
    solver = Solver(problem)
    viz = Visualizer(problem, solver)

    # Read input from the command line
    parser = problem.define_command_line_options()
    parser = solver. define_command_line_options(parser)
    args = parser.parse_args()
    problem.init_from_command_line(args)
    solver. init_from_command_line(args)

    # Solve and plot
    solver.solve()
    import matplotlib.pyplot as plt
    #import scitools.std as plt
    plt = viz.plot(plt=plt)
    E = solver.error()
    if E is not None:
```

```
        print 'Error: %.4E' % E
    plt.show()
```

The file `decay_class.py` constitutes a module with the three classes and the `main` function.

Test the understanding.

Implement the problem in Exercise **??** in terms of problem, solver, and visualizer classes. Equip the classes and their methods with doc strings with tests. Also include nose tests.

4.7 Improving the problem and solver classes

The previous `Problem` and `Solver` classes containing parameters soon get much repetitive code when the number of parameters increases. Much of this code can be parameterized and be made more compact. For this purpose, we decide to collect all parameters in a dictionary, `self.prms`, with two associated dictionaries `self.types` and `self.help` for holding associated object types and help strings. Provided a problem, solver, or visualizer class defines these three dictionaries in the constructor, using default or user-supplied values of the parameters, we can create a super class `Parameters` with general code for defining command-line options and reading them as well as methods for setting and getting a parameter. A `Problem` or `Solver` class will then inherit command-line functionality and the set/get methods from the `Parameters` class.

A generic class for parameters. A simplified version of the parameter class looks as follows:

```
class Parameters:
    def set(self, **parameters):
        for name in parameters:
            self.prms[name] = parameters[name]

    def get(self, name):
        return self.prms[name]

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()

        for name in self.prms:
            tp = self.types[name] if name in self.types else str
            help = self.help[name] if name in self.help else None
            parser.add_argument(
                '--' + name, default=self.get(name), metavar=name,
                type=tp, help=help)

        return parser
```

```
    def init_from_command_line(self, args):
        for name in self.prms:
            self.prms[name] = getattr(args, name)
```

The file class_decay_oo.py contains a slightly more advanced version of class Parameters where we in the set and get functions test for valid parameter names and raise exceptions with informative messages if any name is not registered.

The problem class. A class Problem for the problem $u' = -au$, $u(0) = I$, $t \in (0, T]$, with parameters input a, I, and T can now be coded as

```
class Problem(Parameters):
    """
    Physical parameters for the problem u'=-a*u, u(0)=I,
    with t in [0,T].
    """
    def __init__(self):
        self.prms = dict(I=1, a=1, T=10)
        self.types = dict(I=float, a=float, T=float)
        self.help = dict(I='initial condition, u(0)',
                         a='coefficient in ODE',
                         T='end time of simulation')

    def exact_solution(self, t):
        I, a = self.get('I'), self.get('a')
        return I*np.exp(-a*t)
```

The solver class. Also the solver class is derived from class Parameters and works with the prms, types, and help dictionaries in the same way as class Problem. Otherwise, the code is very similar to class Solver in the decay_class.py file:

```
class Solver(Parameters):
    def __init__(self, problem):
        self.problem = problem
        self.prms = dict(dt=0.5, theta=0.5)
        self.types = dict(dt=float, theta=float)
        self.help = dict(dt='time step value',
                         theta='time discretization parameter')

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.get('I'),
            self.problem.get('a'),
            self.problem.get('T'),
            self.get('dt'),
            self.get('theta'))

    def error(self):
        try:
            u_e = self.problem.exact_solution(self.t)
            e = u_e - self.u
            E = np.sqrt(self.get('dt')*np.sum(e**2))
```

```
        except AttributeError:
            E = None
        return E
```

The visualizer class. Class `Visualizer` can be identical to the one in the `decay_class.py` file since the class does not need any parameters. However, a few adjustments in the `plot` method is necessary since parameters are accessed as, e.g., `problem.get('T')` rather than `problem.T`. The details are found in the file `class_decay_oo.py`.

Finally, we need a function that solves a real problem using the classes `Problem`, `Solver`, and `Visualizer`. This function can be just like `main` in the `decay_class.py` file.

The advantage with the `Parameters` class is that it scales to problems with a large number of physical and numerical parameters: as long as the parameters are defined once via a dictionary, the compact code in class `Parameters` can handle any collection of parameters of any size.

5 Performing scientific experiments

Goal.

This section explores the behavior of a numerical method for a differential equation through computer experiments. In particular, it is shown how scientific experiments can be set up and reported. We address the ODE problem

$$u'(t) = -au(t), \quad u(0) = I, \quad t \in (0, T], \tag{5}$$

numerically discretized by the θ-rule:

$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a \Delta t} u^n, \quad u^0 = I\,.$$

Our aim is to plot $u^0, u^1, \ldots, u^N$ together with the exact solution $u_{\mathrm{e}} = Ie^{-at}$ for various choices of the parameters in this numerical problem: I, a, Δt, and θ. We are especially interested in how the discrete solution compares with the exact solution when the Δt parameter is varied and θ takes on the three values corresponding to the Forward Euler, Backward Euler, and Crank-Nicolson schemes ($\theta = 0, 1, 0.5$, respectively).

5.1 Software

A verified implementation for computing the numerical solution u^n and plotting it together with the exact solution u_{e} is found in the file `decay_mod.py`. This program admits command-line arguments to specify a series of Δt values and

will run a loop over these values and $\theta = 0, 0.5, 1$. We make a slight edit of how the plots are designed: the numerical solution is specified with line type `'r-o'` (dashed red lines with dots at the mesh points), and the `show()` command is removed to avoid a lot of plot windows popping up on the computer screen (but hardcopies of the plot are still stored in files via `savefig`). The slightly modified program has the name `experiments/decay_mod.py`. All files associated with the scientific investigation are collected in a subdirectory `experiments`.

Running the experiments is easy since the `decay_mod.py` program already has the loops over θ and Δt implemented. An experiment with $I = 1$, $a = 2$, $T = 5$, and $dt = 0.5, 0.25, 0.1, 0.05$ is run by

```
Terminal> python decay_mod.py --I 1 --a 2 --makeplot \
          --T 5 --dt 0.5 0.25 0.1 0.05
```

5.2 Combining plot files

The `decay_mod.py` program generates a lot of image files, e.g., `FE_*.png`, `BE_*.png`, and `CN_*.png`. We want to combine all the `FE_*.png` files in a table fashion in one file, with two images in each row, starting with the largest Δt in the upper left corner and decreasing the value as we go to the right and down. This can be done using the `montage` program. The often occurring white areas around the plots can be cropped away by the `convert -trim` command. The remaining white can be made transparent for HTML pages with a non-white background by the command `convert -transparent white`.

Also plot files in the PDF format with names `FE_*.pdf`, `BE_*.pdf`, and `CN_*.pdf` are generated and these should be combined using other tools: `pdftk` to combine individual plots into one file with one plot per page, and `pdfnup` to combine the pages into a table with multiple plots per page. The resulting image often has some extra surrounding white space that can be removed by the `pdfcrop` program. The code snippets below contain all details about the usage of `montage`, `convert`, `pdftk`, `pdfnup`, and `pdfcrop`.

Running manual commands is boring, and errors may easily sneak in. Both for automating manual work and documenting the operating system commands we actually issued in the experiment, we should write a *script* (little program). An alternative is to write the commands into an IPython notebook and use the notebook as the script. A plain script as a standard Python program in a separate text file will be used here.

Reproducible science.

A script that automates running our computer experiments will ensure that the experiments can easily be rerun by ourselves or others in the future, either to check the results or redo the experiments with other input data. Also, whatever we did to produce the results is documented in every detail

in the script. Automating scripts are therefore essential to making our research *reproducible*, which is a fundamental principle in science.

The script takes a list of Δt values on the command line as input and makes three combined images, one for each θ value, displaying the quality of the numerical solution as Δt varies. For example,

```
Terminal> python decay_exper0.py 0.5 0.25 0.1 0.05
```

results in images `FE.png`, `CN.png`, `BE.png`, `FE.pdf`, `CN.pdf`, and `BE.pdf`, each with four plots corresponding to the four Δt values. Each plot compares the numerical solution with the exact one. The latter image is shown in Figure 2.

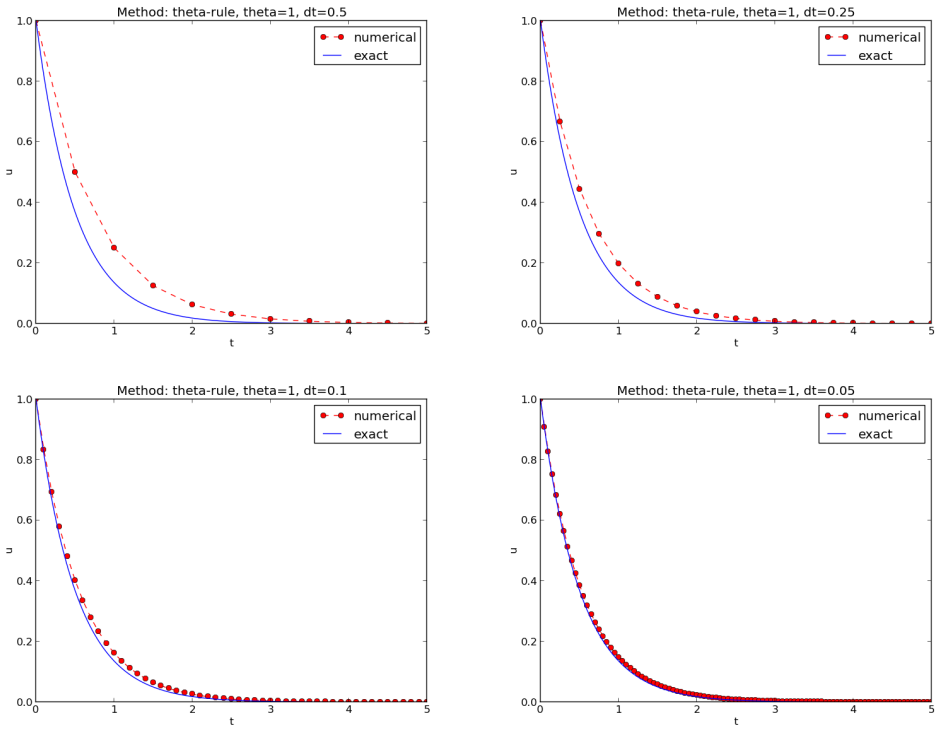


Figure 2: Illustration of the Backward Euler method for four time step values.

Ideally, the script should be scalable in the sense that it works for any number of Δt values, which is the case for this particular implementation:

```
import os, sys

def run_experiments(I=1, a=2, T=5):
    # The command line must contain dt values
    if len(sys.argv) > 1:
        dt_values = [float(arg) for arg in sys.argv[1:]]
    else:
        print 'Usage: %s dt1 dt2 dt3 ...' %  sys.argv[0]
        sys.exit(1)  # abort

    # Run module file as a stand-alone application
    cmd = 'python decay_mod.py --I %g --a %g --makeplot --T %g' % \
          (I, a, T)
    dt_values_str = ' '.join([str(v) for v in dt_values])
    cmd += ' --dt %s' % dt_values_str
    print cmd
    failure = os.system(cmd)
    if failure:
        print 'Command failed:', cmd; sys.exit(1)

    # Combine images into rows with 2 plots in each row
    image_commands = []
    for method in 'BE', 'CN', 'FE':
        pdf_files = ' '.join(['%s_%g.pdf' % (method, dt)
                              for dt in dt_values])
        png_files = ' '.join(['%s_%g.png' % (method, dt)
                              for dt in dt_values])
        image_commands.append(
            'montage -background white -geometry 100%' +
            ' -tile 2x %s %s.png' % (png_files, method))
        image_commands.append(
            'convert -trim %s.png %s.png' % (method, method))
        image_commands.append(
            'convert %s.png -transparent white %s.png' %
            (method, method))
        image_commands.append(
            'pdftk %s output tmp.pdf' % pdf_files)
        num_rows = int(round(len(dt_values)/2.0))
        image_commands.append(
            'pdfnup --nup 2x%d tmp.pdf' % num_rows)
        image_commands.append(
            'pdfcrop tmp-nup.pdf %s.pdf' % method)

    for cmd in image_commands:
        print cmd
        failure = os.system(cmd)
        if failure:
            print 'Command failed:', cmd; sys.exit(1)

    # Remove the files generated above and by decay_mod.py
    from glob import glob
    filenames = glob('*_*.png') + glob('*_*.pdf') + \
                glob('*_*.eps') + glob('tmp*.pdf')
    for filename in filenames:
        os.remove(filename)

if __name__ == '__main__':
    run_experiments()
```

This file is available as `experiments/decay_exper0.py`.

We may comment upon many useful constructs in this script:

- `[float(arg) for arg in sys.argv[1:]]` builds a list of real numbers from all the command-line arguments.
- `failure = os.system(cmd)` runs an operating system command, e.g., another program. The execution is successful only if `failure` is zero.
- Unsuccessful execution usually makes it meaningless to continue the program, and therefore we abort the program with `sys.exit(1)`. Any argument different from 0 signifies to the computer's operating system that our program stopped with a failure.
- `['%s_%s.png' % (method, dt) for dt in dt_values]` builds a list of filenames from a list of numbers (`dt_values`).
- All `montage`, `convert`, `pdftk`, `pdfnup`, and `pdfcrop` commands for creating composite figures are stored in a list and later executed in a loop.
- `glob('*_*.png')` returns a list of the names of all files in the current directory where the filename matches the Unix wildcard notation `*_*.png` (meaning any text, underscore, any text, and then `.png`).
- `os.remove(filename)` removes the file with name `filename`.

5.3 Interpreting output from other programs

Programs that run other programs, like `decay_exper0.py` does, will often need to interpret output from those programs. Let us demonstrate how this is done in Python by extracting the relations between θ, Δt, and the error E as written to the terminal window by the `decay_mod.py` program, when being executed by `decay_exper0.py`. We will

- read the output from the `decay_mod.py` program
- interpret this output and store the E values in arrays for each θ value
- plot E versus Δt, for each θ, in a log-log plot

The simple `os.system(cmd)` call does not allow us to read the output from running `cmd`. Instead we need to invoke a bit more involved procedure:

```
from subprocess import Popen, PIPE, STDOUT
p = Popen(cmd, shell=True, stdout=PIPE, stderr=STDOUT)
output, dummy = p.communicate()
failure = p.returncode
if failure:
    print 'Command failed:', cmd; sys.exit(1)
```

The command stored in `cmd` is run and all text that is written to the standard output *and* the standard error is available in the string `output`. Or in other words, the text in `output` is what appeared in the terminal window while running `cmd`.

Our next task is to run through the `output` string, line by line, and if the current line prints θ, Δt, and E, we split the line into these three pieces and store the data. The chosen storage structure is a dictionary `errors` with keys `dt` to hold the Δt values in a list, and three θ keys to hold the corresponding E values in a list. The relevant code lines are

```
errors = {'dt': dt_values, 1: [], 0: [], 0.5: []}
for line in output.splitlines():
    words = line.split()
    if words[0] in ('0.0', '0.5', '1.0'):  # line with E?
        # typical line: 0.0   1.25:    7.463E+00
        theta = float(words[0])
        E = float(words[2])
        errors[theta].append(E)
```

Note that we do not bother to store the Δt values as we read them from `output`, because we already have these values in the `dt_values` list.

We are now ready to plot E versus Δt for $\theta = 0, 0.5, 1$:

```
import matplotlib.pyplot as plt
plt.loglog(errors['dt'], errors[0], 'ro-')
plt.hold('on')
plt.loglog(errors['dt'], errors[0.5], 'b+-')
plt.loglog(errors['dt'], errors[1], 'gx-')
plt.legend(['FE', 'CN', 'BE'], loc='upper left')
plt.xlabel('log(time step)')
plt.ylabel('log(error)')
plt.title('Error vs time step')
plt.savefig('error.png')
plt.savefig('error.pdf')
```

Plots occasionally need some manual adjustments. Here, the axis of the log-log plot look nicer if we adapt them strictly to the data, see Figure 3. To this end, we need to compute $\min E$ and $\max E$, and later specify the extent of the axes:

```
# Find min/max for the axis
E_min = 1E+20; E_max = -E_min
for theta in 0, 0.5, 1:
    E_min = min(E_min, min(errors[theta]))
    E_max = max(E_max, max(errors[theta]))

plt.loglog(errors['dt'], errors[0], 'ro-')
...
plt.axis([min(dt_values), max(dt_values), E_min, E_max])
...
```

The complete program, incorporating the code snippets above, is found in `experiments/decay_exper1.py`. This example can hopefully act as template for numerous other occasions where one needs to run experiments, extract data

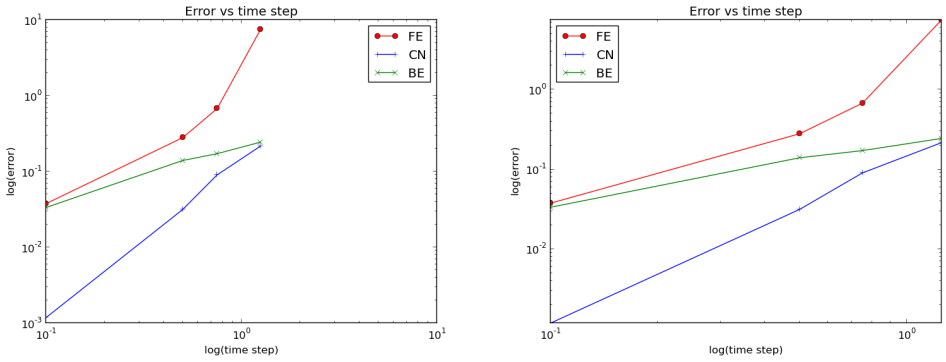


Figure 3: Default plot (left) and manually adjusted axes (right).

from the output of programs, make plots, and combine several plots in a figure file. The `decay_exper1.py` program is organized as a module, and other files can then easily extend the functionality, as illustrated in the next section.

5.4 Making a report

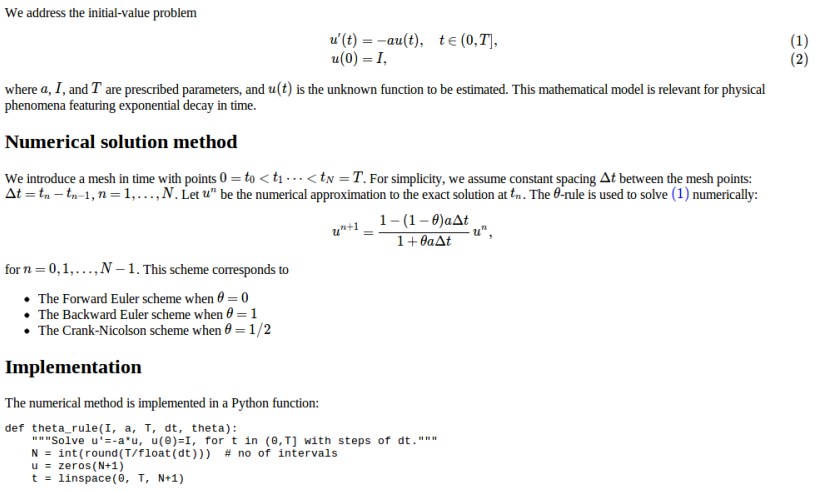
The results of running computer experiments are best documented in a little report containing the problem to be solved, key code segments, and the plots from a series of experiments. At least the part of the report containing the plots should be automatically generated by the script that performs the set of experiments, because in that script we know exactly which input data that were used to generate a specific plot, thereby ensuring that each figure is connected to the right data. Take a look at an example at `http://tinyurl.com/k3sdbuv/writing_reports//sphinx-cloud/` to see what we have in mind.

Plain HTML. Scientific reports can be written in a variety of formats. Here we begin with the HTML format which allows efficient viewing of all the experiments in any web browser. The program `decay_exper1_html.py` calls `decay_exper1.py` to perform the experiments and then runs statements for creating an HTML file with a summary, a section on the mathematical problem, a section on the numerical method, a section on the `solver` function implementing the method, and a section with subsections containing figures that show the results of experiments where Δt is varied for $\theta = 0, 0.5, 1$. The mentioned Python file contains all the details for writing this HTML report. You can view the report on `http://tinyurl.com/k3sdbuv/writing_reports//_static/report_html.html`.

HTML with MathJax. Scientific reports usually need mathematical formulas and hence mathematical typesetting. In plain HTML, as used in the `decay_exper1_html.py` file, we have to use just the keyboard characters to

write mathematics. However, there is an extension to HTML, called MathJax, which allows formulas and equations to be typeset with LaTeX syntax and nicely rendered in web browsers, see Figure 4. A relatively small subset of LaTeX environments is supported, but the syntax for formulas is quite rich. Inline formulas are look like `\( u'=-au \)` while equations are surrounded by `$$` signs. Inside such signs, one can use `\[ u'=-au \]` for unnumbered equations, or `\begin{equation}` and `\end{equation}` surrounding `u'=-au` for numbered equations, or `\begin{align}` and `\end{align}` for multiple aligned equations. You need to be familiar with mathematical typesetting in LaTeX.

The file `decay_exper1_mathjax.py` contains all the details for turning the previous plain HTML report into web pages with nicely typeset mathematics. The corresponding HTML code be studied to see all details of the mathematical typesetting.



We address the initial-value problem

$$u'(t) = -au(t), \quad t \in (0,T], \tag{1}$$
$$u(0) = I, \tag{2}$$

where a, I, and T are prescribed parameters, and $u(t)$ is the unknown function to be estimated. This mathematical model is relevant for physical phenomena featuring exponential decay in time.

Numerical solution method

We introduce a mesh in time with points $0 = t_0 < t_1 \cdots < t_N = T$. For simplicity, we assume constant spacing Δt between the mesh points: $\Delta t = t_n - t_{n-1}$, $n = 1, \ldots, N$. Let u^n be the numerical approximation to the exact solution at t_n. The θ-rule is used to solve (1) numerically:

$$u^{n+1} = \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}\, u^n,$$

for $n = 0, 1, \ldots, N-1$. This scheme corresponds to

- The Forward Euler scheme when $\theta = 0$
- The Backward Euler scheme when $\theta = 1$
- The Crank-Nicolson scheme when $\theta = 1/2$

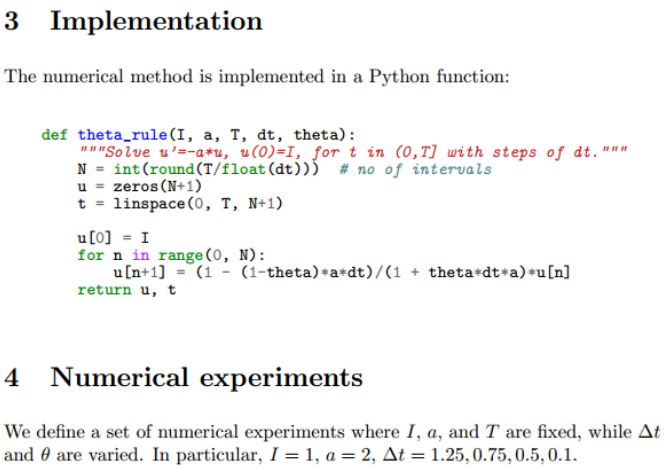
Implementation

The numerical method is implemented in a Python function:

```
def theta_rule(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    N = int(round(T/float(dt)))  # no of intervals
    u = zeros(N+1)
    t = linspace(0, T, N+1)
```

Figure 4: Report in HTML format with MathJax.

LaTeX. The *de facto* language for mathematical typesetting and scientific report writing is LaTeX. A number of very sophisticated packages have been added to the language over a period of three decades, allowing very fine-tuned layout and typesetting. For output in the PDF format, see Figure 5 for an example, LaTeX is the definite choice when it comes to quality. The LaTeX language used to write the reports has typically a lot of commands involving backslashes and braces. For output on the web, using HTML (and not the PDF directly in the browser window), LaTeX struggles with delivering high quality typesetting. Other tools, especially Sphinx, give better results and can also produce nice-looking PDFs. The file `decay_exper1_latex.py` shows how to generate the LaTeX source from a program.



3 Implementation

The numerical method is implemented in a Python function:

```
def theta_rule(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    N = int(round(T/float(dt)))  # no of intervals
    u = zeros(N+1)
    t = linspace(0, T, N+1)

    u[0] = I
    for n in range(0, N):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

4 Numerical experiments

We define a set of numerical experiments where I, a, and T are fixed, while Δt and θ are varied. In particular, $I = 1$, $a = 2$, $\Delta t = 1.25, 0.75, 0.5, 0.1$.

Figure 5: Report in PDF format generated from LaTeX source.

Sphinx. Sphinx is a typesetting language with similarities to HTML and LaTeX, but with much less tagging. It has recently become very popular for software documentation and mathematical reports. Sphinx can utilize LaTeX for mathematical formulas and equations (via MathJax or PNG images). Unfortunately, the subset of LaTeX mathematics supported is less than in full MathJax (in particular, numbering of multiple equations in an `align` type environment is not supported). The Sphinx syntax is an extension of the reStructuredText language. An attractive feature of Sphinx is its rich support for fancy layout of web pages. In particular, Sphinx can easily be combined with various layout *themes* that give a certain look and feel to the web site and that offers table of contents, navigation, and search facilities, see Figure 6.

Markdown. A recently popular format for easy writing of web pages is Markdown. Text is written very much like one would do in email, using spacing and special characters to naturally format the code instead of heavily tagging the text as in LaTeX and HTML. With the tool Pandoc one can go from Markdown to a variety of formats. HTML is a common output format, but LaTeX, epub, XML, OpenOffice, MediaWiki, and MS Word are some other possibilities.

Wiki formats. A range of wiki formats are popular for creating notes on the web, especially documents which allow groups of people to edit and add content. Apart from MediaWiki (the wiki format used for Wikipedia), wiki formats have no support for mathematical typesetting and also limited tools for displaying computer code in nice ways. Wiki formats are therefore less suitable for scientific reports compared to the other formats mentioned here.

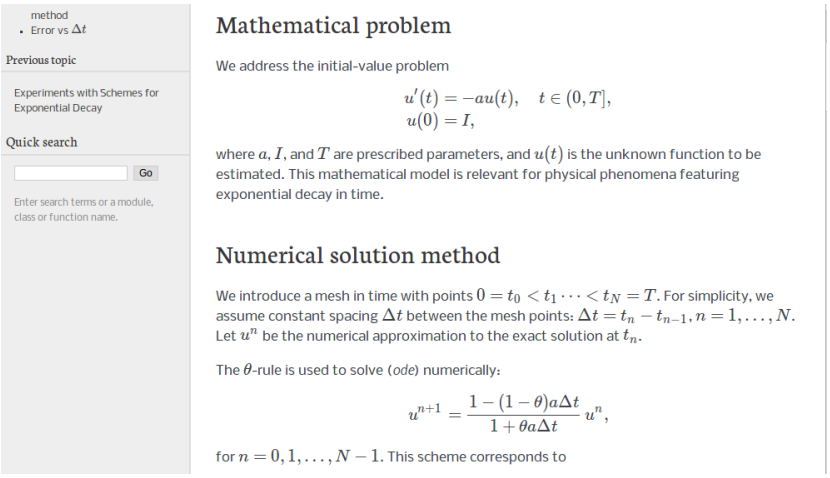


Figure 6: Report in HTML format generated from Sphinx source.

DocOnce. Since it is difficult to choose the right tool or format for writing a scientific report, it is advantageous to write the content in a format that easily translates to LaTeX, HTML, Sphinx, Markdown, and various wikis. DocOnce is such a tool. It is similar to Pandoc, but offers some special convenient features for writing about mathematics and programming. The tagging is modest, somewhere between LaTeX and Markdown. The program `decay_exper_do.py` demonstrates how to generate (and write) DocOnce code for a report.

Worked example. The HTML, LaTeX (PDF), Sphinx, and DocOnce formats for the scientific report whose content is outlined above, are exemplified with source codes and results at the web pages associated with this teaching material: `http://tinyurl.com/k3sdbuv/writing_reports/`.

5.5 Publishing a complete project

A report documenting scientific investigations should be accompanied by all the software and data used for the investigations so that others have a possibility to redo the work and assess the qualify of the results. This possibility is important for *reproducible research* and hence reaching reliable scientific conclusions.

One way of documenting a complete project is to make a directory tree with all relevant files. Preferably, the tree is published at some project hosting site like Bitbucket, GitHub, or Googlecode so that others can download it as a tarfile, zipfile, or clone the files directly using a version control system like Mercurial or Git. For the investigations outlined in Section 5.4, we can create a directory tree with files

```
setup.py
./src:
   decay_mod.py
```

```
./doc:
   ./src:
      decay_exper1_mathjax.py
      make_report.sh
      run.sh
   ./pub:
      report.html
```

The `src` directory holds source code (modules) to be reused in other projects, the `setup.py` builds and installs such software, the `doc` directory contains the documentation, with `src` for the source of the documentation and `pub` for ready-made, published documentation. The `run.sh` file is a simple Bash script listing the `python` command we used to run `decay_exper1_mathjax.py` to generate the experiments and the `report.html` file.

6 Exercises

Exercise 1: Refactor a flat program in terms of a function

For simple ODEs of the form

$$u' = f(t), \quad u(0) = I, \ t \in (0, T]$$

we can find the solution by straightforward integration:

$$u(t) = \int_0^t f(\tau) d\tau \, .$$

To compute $u(t)$ for $t \in [0, T]$, we introduce a uniform time mesh with points $t_n = n\Delta t$ and apply to Trapezoidal rule to approximate the integral. Suppose we have computed the numerical approximation u^n to $u(t_n)$. We have

$$u(t_{n+1}) = u(t_n) + \int_{t_n}^{t_{n+1}} f(\tau) d\tau \, .$$

Using the Trapezoidal rule we get

$$u^{n+1} = u^n + \frac{1}{2}\Delta t(f(t_n) + f(t_{n+1})) \, . \tag{6}$$

The starting value is $u^0 = I$. A corresponding implementation for the case $f(t) = 2t + 1$ is given next.

```
# f(t) is 2*t + 1
T = 2
from numpy import *
dt = 0.2                # time step
Nt = int(round(T/dt))  # no of mesh points
u = zeros(Nt+1)
t = linspace(0, T, Nt+1)
for n in range(Nt-1):
    u[n+1] = u[n] + 0.5*dt*(2*t[n]+1 + 2*t[n+1]+1)
```

This is a flat program. Refactor the program as a function `solver(f, I, T, dt)`, where `f` is the Python implementation of the mathematical function $f(t)$ that is to be integrated. The return value of `solver` is the pair (`u`, `t`) representing the solution values and the associated time mesh. Filename: `integrate.py`.

Remarks. Many prefer to do a first implementation of an algorithm as a flat program and hardcode formulas, here the $f(t)$, into the algorithm. Unfortunately, this coding style makes it difficult to reuse a well-tested algorithm. When the flat program works, it is strongly recommended to *refactor* the code (i.e., rearrange the statements) such that general algorithms are encapsulated in Python functions. The function arguments should be chosen such that the function can be applied for a large class of problems, here all problems that can be expressed as $u' = f(t)$,.

Exercise 2: Compare methods for a given time mesh

Make a program that imports the `solver` function from the `decay_mod` module and offers a function `compare(dt, I, a)` for comparing, in a plot, the methods corresponding to $\theta = 0, 0.5, 1$ and the exact solution. This plot shows the accuracy of the methods for a given time mesh. Read input data for the problem from the command line using appropriate functions in the `decay_mod` module (the `-dt` option for giving several time step values can be reused: just use the first time step value for the computations). Filename: `decay_compare_theta.py`.

Problem 3: Write a doctest

Type in the following program and equip the `roots` function with a doctest:

```
import sys
# This sqrt(x) returns real if x>0 and complex if x<0
from numpy.lib.scimath import sqrt

def roots(a, b, c):
    """
    Return the roots of the quadratic polynomial
    p(x) = a*x**2 + b*x + c.

    The roots are real or complex objects.
    """
    q = b**2 - 4*a*c
    r1 = (-b + sqrt(q))/(2*a)
    r2 = (-b - sqrt(q))/(2*a)
    return r1, r2

a, b, c = [float(arg) for arg in sys.argv[1:]]
print roots(a, b, c)
```

Make sure to test both real and complex roots. Write out numbers with 14 digits or less. Filename: `doctest_roots.py`.

Problem 4: Write a nose test

Make a nose test for the `roots` function in Problem 3. Filename: `test_roots.py`.

Problem 5: Make a module

Let

$$q(t) = \frac{RAe^{at}}{R + A(e^{at} - 1)}\,.$$

Make a Python module `q_module` containing two functions `q(t)` and `dqdt(t)` for computing $q(t)$ and $q'(t)$, respectively. Perform a `from numpy import *` in this module. Import `q` and `dqdt` in another file using the "star import" construction `from q_module import *`. All objects available in this file is given by `dir()`. Print `dir()` and `len(dir())`. Then change the import of `numpy` in `q_module.py` to `import numpy as np`. What is the effect of this import on the number of objects in `dir()` in a file that does `from q_module import *`? Filename: `q_module.py`.

Exercise 6: Make use of a class implementation

We want to solve the exponential decay problem $u' = -au$, $u(0) = I$, for several Δt values and $\theta = 0, 0.5, 1$. For each Δt value, we want to make a plot where the three solutions corresponding to $\theta = 0, 0.5, 1$ appear along with the exact solution. Write a function `experiment` to accomplish this. The function should import the classes `Problem`, `Solver`, and `Visualizer` from the `decay_class` module and make use of these. A new command-line option `--dt_values` must be added to allow the user to specify the Δt values on the command line (the options `-dt` and `-theta` implemented by the `decay_class` module have then no effect when running the `experiment` function). Note that the classes in the `decay_class` module should *not* be modified. Filename: `decay_class_exper.py`.

Exercise 7: Generalize a class implementation

Consider the file `decay_class.py` where the exponential decay problem $u' = -au$, $u(0) = I$, is implemented via the classes `Problem`, `Solver`, and `Visualizer`. Extend the classes to handle the more general problem

$$u'(t) = -a(t)u(t) + b(t), \quad u(0) = I,\ t \in (0, T],$$

using the θ-rule for discretization.

In the case with arbitrary functions $a(t)$ and $b(t)$ the problem class is no longer guaranteed to provide an exact solution. Let the `u_exact` in class `Problem` return `None` if the exact solution for the particular problem is not available. Modify classes `Solver` and `Visualizer` accordingly.

Add test functions `test_*()` for the nose testing tool in the module. Also add a demo example where the environment suddenly changes (modeled as an

abrupt change in the decay rate a):

$$a(t) = \begin{cases} 1, & 0 \leq t \leq t_p, \\ k, & t > t_p, \end{cases}$$

where t_p is the point of time the environment changes. Take $t_p = 1$ and make plots that illustrate the effect of having $k \gg 1$ and $k \ll 1$. Filename: `decay_class2.py`.

Exercise 8: Generalize an advanced class implementation

Solve Exercise 7 by utilizing the class implementations in `decay_class_oo.py`. Filename: `decay_class3.py`.

References

[1] H. P. Langtangen. *A Primer on Scientific Programming With Python*. Texts in Computational Science and Engineering. Springer, third edition, 2012.

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